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Graphical Interface for the Physics-Based Generation of Inputs to 3D MEEC SGEMP and SREMP Simulations

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GRAPHICAL INTERFACE FOR THE PHYSICS-BASED GENERATION OF INPUTS TO 3D MEEC SGEMP AND SREMP SIMULATIONS†

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ABSTRACT

A graphical user interface (GUI) is under development for the MEEC family of SGEMP and SREMP simulation codes [1,2]. These codes are “workhorse” legacy codes that have been in use for nearly two decades, with modifications and enhanced physics models added throughout the years. The MEEC codes are currently being evaluated for use by the DOE in the Dual Revalidation Program and experiments at NIF. The new GUI makes the codes more accessible and less prone to input errors by automatically generating the parameters and grids that previously had to be designed “by hand”. Physics-based algorithms define the simulation volume with expanding meshes. Users are able to specify objects, materials, and emission surfaces through dialogs and input boxes. 3D and orthographic views are available to view objects in the volume. Zone slice views are available for stepping through the overlay of objects on the mesh in planes aligned with the primary axes.

BACKGROUND

The MEEC codes are self-consistent particle-pushing codes that solve the Maxwell electromagnetic equations and Lorentz particle equations using standard finite-difference methods. These codes have been used successfully in the past to model SGEMP and SREMP problems for UGT and AGT experiments. Depending on the environment (vacuum, thin air, dense air) and geometry (2D or 3D), one of nine versions is employed.

In recent years, the nine versions of MEEC had been transitioned from mainframe versions to versions that can run on workstations or high-end PCs. What had been lacking until now was an easy and intuitive way to use the codes and to check the input. Building the MEEC input "by hand" typically involved many hours experienced analysts' time. Verification of an acceptable input file was supported only by a very simple plotted display of zone and object location.

Visualization aids were needed to allow analysts to verify correct object and source locations. Also needed was an automatic mesh generator that could incorporate the physics constraints on meshing the simulation volume well enough to model the SGEMP sources and the coupling to systems.

GRAPHICAL USER INTERFACE

We have used Visual Basic 5 for Windows 32 bit development to create the interface. VB was used because it is the most scalable language to build an application. The support for the language and available tools reduce the development time, and the VB 5 environment allows for developing rich, object-oriented code, as well as on-the-fly debugging. 3D display algorithms were adapted from Stevens [3].

The GUI consists of 1 main form, 4 modules, 5 dialogs, and 8 classes. Figure 1 shows one of the screens, including the main drawing window to the right and a listbar to the left. A click on the listbar title unfolds a topic, e.g. Sources & Boundaries, Objects & Materials, etc. Initial inputs are the simulation boundaries. The pop-up dialog window shown in Figure 1 currently requires users to specify the emission current and average electron energy. One of the key upgrades now in progress will include a link to the CEPXS/ONEBFP radiation transport code to give users the option of an accurately computed set of emission currents [4]. The emission levels are defined here so that they can be assigned to the surfaces of objects, as indicated in Figure 2.

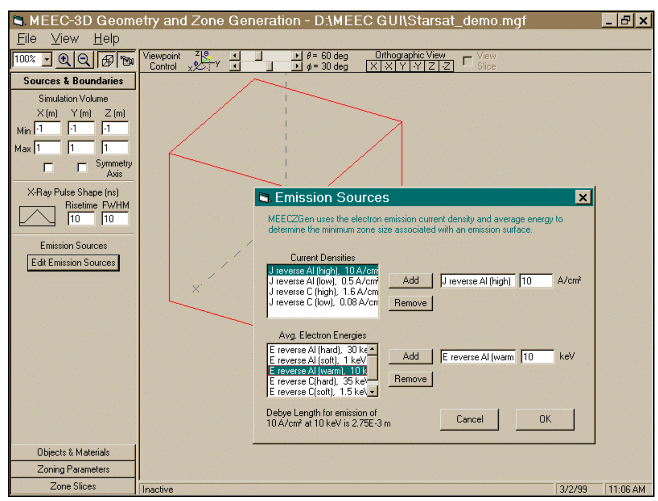

Figure 1. Example screen for simulation boundaries and dialog for specifying SGEMP emission currents.

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Figure 2 has a wire frame of an example satellite in the main drawing window and the dialog shows the emission surfaces that the user has assigned to the center body object. Note that the two surfaces that have been selected as emission surfaces are marked as such by the program, which applies hash marks to the surfaces. Simple shapes such as boxes, planes, rods and wires can be selected and sized for dielectric, metal and lossy (finite conductivity) objects. [Other simple object shapes, such as cones and frustums, are planned added for the next upgrade. Also, MEEC itself will be modified in the next phase of the project so that it can accept a simple, single-line input definition for curved objects, internally generating the same objects on the mesh as shown by the GUI.]

Users may specify several types of materials by setting different property values for each one, including name and display color.

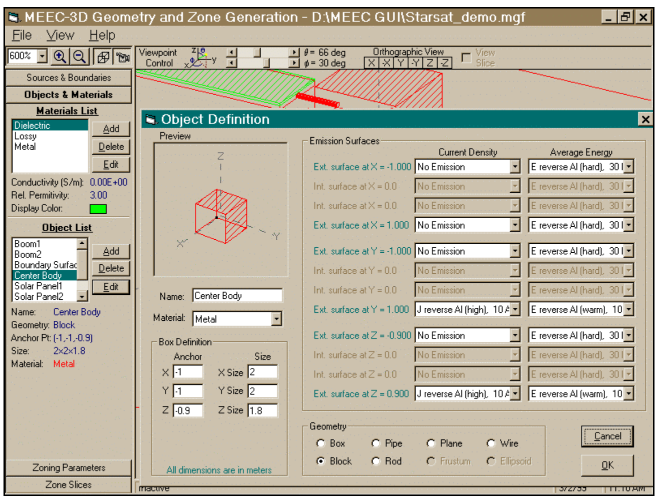

Figure 2. Object wire frame display and assignment of emission surfaces.

Figure 3 shows the 3D display of the simulation satellite with surface color turned on. Controls at the top of the window allow the view to be rotated to an arbitrary viewing angle and zoomed in or out. When the display is set to orthographic view (aligned with an axis, as in Figure 3), the cartesian coordinates appear on the status bar to let users check object positions by pointing at them with the mouse.

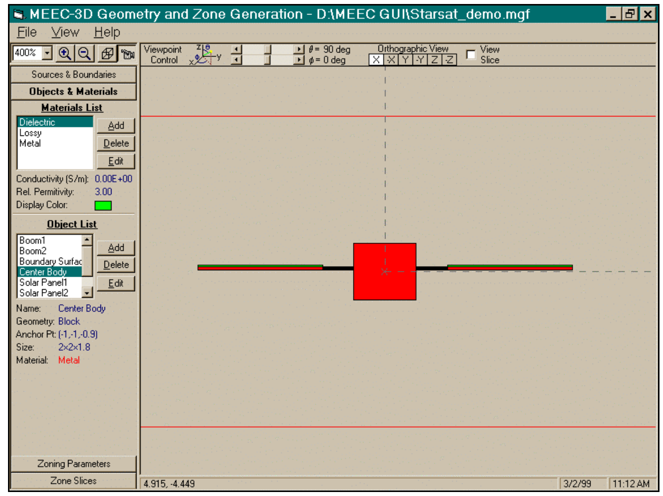

Figure 3. 3D display of user-defined objects in simulation volume.

MESH GENERATOR

We have developed algorithms for generating the cartesian grid. The algorithm defines zones along each axis, from one object surface to another, taking care to make zones sufficiently small near emission surfaces. For example, vacuum SGEMP simulation requires resolving the space charge that builds up in a layer of thickness λ_{SCL} next to an emission surface [5]:

$$\lambda_{SCL} = \left(\varepsilon_0 \sqrt{\frac{e}{8 m_e \pi}} \frac{E_e^{3/2}}{J_e} \right)^{1/2} \qquad (1)$$

[space-charge-limited charge cloud thickness]

where E_e is the average electron energy (in eV), J_e is the emission current density (in A/m^2), and constants are in MKS units.

To model less intense SGEMP or IEMP that has little or no space-charge limiting, the characteristic thickness of the charge layer is set by whichever is smaller - the distance an emitted charge cloud can travel during the time to emit change or the full length of the simulation volume:

$$\lambda_{lin} = \min(v_e T_w, L) \qquad (2)$$

[linear limit for emitted charge cloud thickness]

where T_W is the x-ray pulse full-width-at-half-maximum (in seconds) and L is the distance across the simulation volume). Choices for E_e and J_e are available from standard references and simple PC codes, or, as is planned in the next MEEC GUI upgrade, these quantities can be computed by accurate transport codes.

The mesh algorithm uses the lesser of the results of equations 1 and 2, using fine zones ($\lambda/3$) near the emission surface. It is necessary to use more than one zone to self-consistently model the motion of electrons that are pulled back to the emission surface by intense electric fields. The time step for the simulation is strictly constrained by the need to resolve wave propagation across the smallest cells (Courant condition, required for stability):

$$\Delta t \le \frac{\Delta x_{min}}{\sqrt{3}c} \qquad (3)$$

Grid expansion rates default to a reasonably low value of 1.4 to minimize numerical dispersion of the propagated electromagnetic fields generated in the region of interest. An upper bound to the cell size is set by the requirement that the mesh resolve the characteristic frequency of electromagnetic fields induced in the volume. This is accomplished by having grid lengths about 1/8 the wavelength. The rise time of the E field is used to define the highest frequency of interest. The largest grid dimension should be:

$$\Delta x_{max} = ct_R/8 \qquad (4)$$

where t_R is the response rise time, the smaller of two values – the x-ray pulse rise time, T_R, and the time to space-charge limit:

$$t_R = \min\left(T_R, \left(\frac{5.7\varepsilon_0 m_e v_e T_R}{eJ_e}\right)^{1/3}\right) \qquad (5)$$

Figure 4 plots this rise time for the emission from aluminum. Note the dots on the chart, which indicate the variation in both J and t_R at several blackbody temperatures for an example of 1 cal/cm^2 fluence. At high fluence and/or low blackbody temperatures, a sub-nanosecond rise time results. In such cases, the largest recommended grid size is under 10 cm and the number of simulation zones grows accordingly.

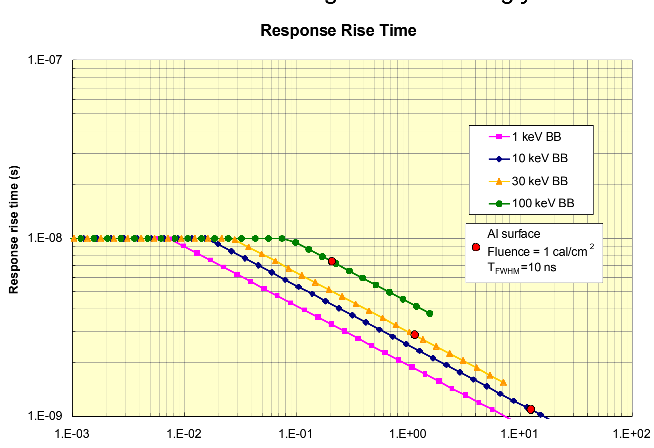

Figure 4. Characteristic time for SGEMP response.

Currents and quasi-static E fields generated on the objects are of highest interest for SGEMP problems. In large simulation volumes, the total number of zones becomes unmanageably large unless equation 4 is relaxed to larger Δx_{max} in regions far from the objects of interest. Users are able to override the default maximum grid size and growth rates for this reason.

Figure 5 shows example mesh generator results for a high fluence case of 10 keV blackbody on an aluminum satellite. The code-generated mesh is shown referenced to the surfaces defined at grid edges. Users may make changes to zone sizes and growth rate in each sub-region and observe the results in the autogenerated mesh and total zone number. Note from Figure 5 that object boundaries occur at the minimum of the zone size curve (solid line). The grid is expanded away from these surfaces in both directions using the specified growth rate. This strategy keeps small zones near object surfaces. Constant zones can be specified, if desired. The code prevents overrides of the maximum growth rate and issues warnings if the spacecharge barrier is not adequately resolved.

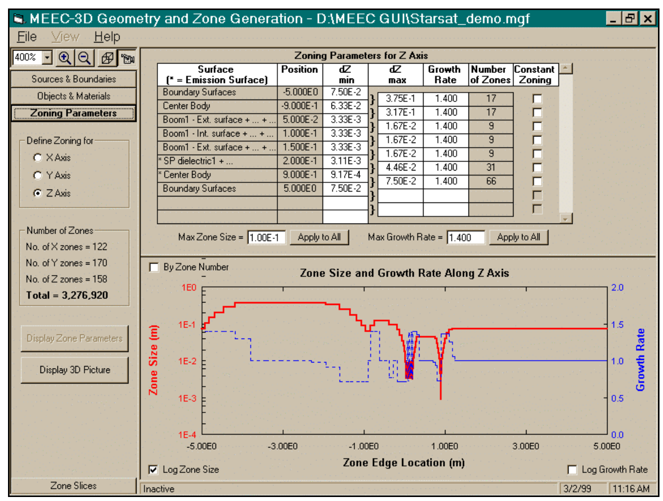

Figure 5. Mesh generation results for a sample problem.

One can quickly use the dialog options to trade off mesh fineness with number of zones, for example reducing the 3 million zones generated in Figure 5 to a more managable 1.1 million in Figure 6.

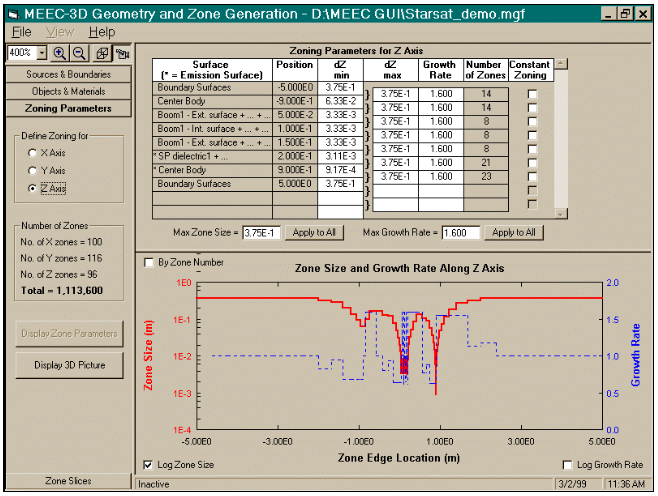

Figure 6. Example of a coarser mesh due to user override of the maximum zone size and growth rate.

Figure 7 illustrates the zone slice view that allows users to step through each layer of the simulation mesh, examining the placement of object boundaries and output requests, i.e. fields or currents developed at that zone. The user is able to pan through the simulation slice looking at a 15 x 15 zone section. This section is outlined on a thumbnail picture in the right side of the window to reference the section to the slice through the entire simulation volume.

```
Satellite demo, 2 planes of symmetry, square cross section boom
10 KeV BB source to get reverse electrons from Al and C
*
MAXWELL CIRCUIT
GEOMETRY = CARTESIAN
X SYMMETRY
Y SYMMETRY
X ZONING = -6.00000E+00, -5.75000E+00, -5.50000E+00, -5.25000E+00, /
           -5.00000E+00, -4.75000E+00, -4.50000E+00, -4.25000E+00, /
           -4.00000E+00, -3.75000E+00, -3.50000E+00, -3.25000E+00, /
           -3.00000E+00, -2.75000E+00, -2.50000E+00, -2.25000E+00, /
           -2.00000E+00, -1.75000E+00, -1.53620E+00, -1.34635E+00, /
           -1.21979E+00, -1.13542E+00, -1.07917E+00, -1.04167E+00, /
           -1.01667E+00, -1.00000E+00, -9.83333E-01, -9.58458E-01, /
           -9.21332E-01, -8.84078E-01, -8.28668E-01, -7.91542E-01, /
           -7.66667E-01, -7.50000E-01, -7.33333E-01, -7.08333E-01, /
           -6.70833E-01, -6.14583E-01, -5.30209E-01, -4.03646E-01, /
           -2.99622E-01, -2.14193E-01, -1.57239E-01, -1.19271E-01, /
           -9.39583E-02, -7.70833E-02, -6.58333E-02, -5.83333E-02, /
           -5.33333E-02, -5.00000E-02, -4.66667E-02, -4.16917E-02, /
```

zone edges

…(more zones for x, y, z axes)…

```
* Solar Panel2 of Metal
*
CV ( -7.50000E-01, -6.00000E+00,  5.00000E-02 ) TO /
   ( 7.50000E-01, -2.00000E+00,  1.50000E-01 )
*
* SP dielectric2 of Dielectric
*
DV ( -7.50000E-01, -6.00000E+00,  1.50000E-01 ) TO /
   ( 7.50000E-01, -2.00000E+00,  2.00000E-01 ) EPS = 2.65620E-11
```

conducting volume

dielectric volume

…(more object definitions)…

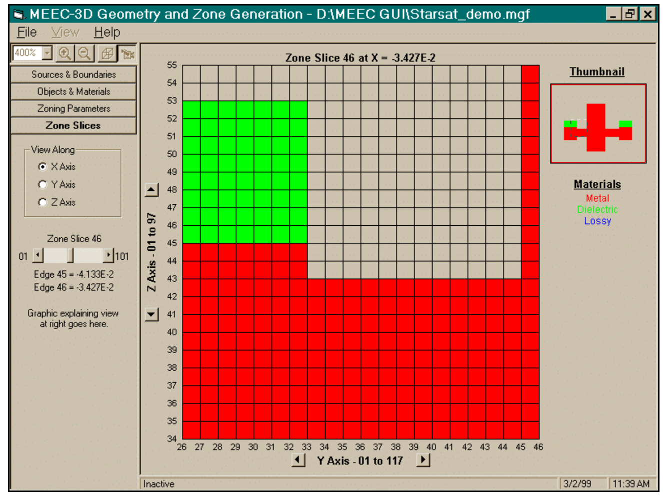

Figure 7. Zone slice view of the satellite example.

As can be seen in Figure 7, the zone slice view is a distorted image of the object because all zones are represented as the same size. In particular, the satellite appears very tall (many zones used near the top emission surface) but the solar panels appear very short (larger zones in the y direction in these regions).

MEEC INPUT FILE

The new MEEC GUI writes a MEEC input file when the problem objects and zoning have been defined to the user's satisfaction. The output file is an ASCII text file with standard key words used by MEEC. Figure 8 indicates a portion of the file generated by the GUI for a variation of simple satellite example that has been described throughout this paper. The GUI prompts the user for header information to identify the file and then writes out the zoning and material definitions. Comment lines (those preceded by asterisks) have also been automatically generated by the GUI to describe the objects as the user has input them through the GUI.

A 3D MEEC view of the meshed objects will be available in future versions so that users can see perspective views of their simulation objects cast onto the 3D mesh.

Note from Figure 8 the keywords X SYMMETRY and Y SYMMETRY. For the test calculation, the simulation size has been reduced by a factor of 4 by employing two planes of symmetry (selected by user). 380,180 total zones are employed. Since the example problem is a very simple perpendicular illumination of the satellite, there are two natural planes of symmetry that occur, and MEEC handles these by applying the appropriate boundary conditions on fields and particles at the mirror planes.

Figure 9 shows the simulation volume employed in the test case that was then run with MEEC. Note that prescribing symmetry planes puts the quarter-satellite in the 3rd quadrant of the XY plane - this is an historical MEEC convention, since the zone numbering starts at the negative positions.

```
RUN CONTROLS
TIME STEP = 1.4E-12
STOP TIME = 30.0E-09
RUN TIME = 500000.0 CPU SECONDS
MAXIMUM PRINT POINTS = 50
MAXIMUM PLOT POINTS = 500
EMITTER TO FIELD RATIO = 1
PUSHER TO FIELD RATIO = 1
MAXIMUM PARTICLES EXCEEDING C = 100
*
WRITE DUMP TAPE DELTA = 500000.0
*                                  Restart file (entire simulation)
SAVE PLOT FILE                     saved at this CPU interval
*
EMISSION CHARACTERISTICS
*
* TIME HISTORY OF 10 NS UP AND 10 NS DOWN
*
EMISSION INTENSITY 1 = 0.0,0.0, 10.0E-09,1.0, 20.0E-09,0.0, PLOT
*
* ENERGY DISTRIBUTION 1 IS FOR REVERSE ELECTRON EMISSION
* FROM 20 MIL AL SURFACE FOR 10 KEV BB - NO SHIELDING
*
* REMEMBER TO INPUT AS DN/DE [(#/MeV/cm2)/(cal/cm2)] VS E (ev)
*
ENERGY DISTRIBUTION 1 = 1.075E+03,1.091E+14,
1.237E+03,1.356E+14, /
            1.423E+03,1.726E+14, 1.636E+03,1.175E+14, /
            1.882E+03,4.280E+13, 2.165E+03,4.277E+13, /
```

… (more energy and angle distributions)…

```
*                       emission direction defined by cross
EMISSION SURFACES       product of change vectors, ΔX  x ΔY
*
*
* AL EMISSION IS FROM THE CENTER BODY IN THE POSITIVE Z
DIRECTION
*
( -1.00, -1.00, 0.90) TO ( -0.90, -1.00, 0.90) TO ( -0.90, -0.90, 0.90) /
INT 1, TIMES 1.00E+05, ED 1, AD 1, ADQ3 3, N = 2
( -0.90, -1.00, 0.90) TO ( -0.80, -1.00, 0.90) TO ( -0.80, -0.90, 0.90) /
INT 1, TIMES 1.00E+05, ED 1, AD 1, ADQ3 3, N = 2
```

(more emission surface definitions)

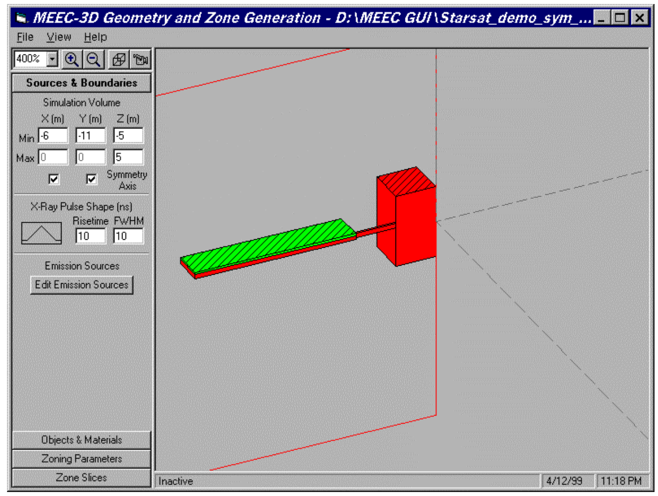

Figure 9. MEEC test simulation employing two symmetry planes.

MEEC TEST SIMULATION USING INPUT FILE GENERATED BY GUI

The partial input file generated by the GUI was taken without any modification and completed by manually adding the remaining portion of the input that deals with the emission surfaces and output requests. Figure 10 shows some of the manual input, indicating the Run Controls (stop time, particle emit and update frequency, etc.) as well as emission surfaces. As for the emission distributions, the next update of the GUI will automatically generate the emission surfaces, one of the most tedious of the remaining inputs. The only significant input not addressed by existing and near term versions of the MEEC GUI is the selection of output requests. This input can be fairly easily composed by using the slice view of the GUI to identify the zones for monitoring fields and currents.

The resulting composite input file was run to demonstrate that a sensible simulation had been designed. The results were highly satisfactory - none of the GUI input had to be redone or even "tweaked". The only factor that greatly affected the quality of the output SGEMP calculation was the number of particles emitted per time step. These numbers, put in by hand at present, are set from past experience. One makes a tradeoff of large particle number and simulation execution time. The number of particles needed to make a "good" simulation, i.e. one not greatly suffering from particle "noise", is bought at the expense oft the time and computer resources needed to run a larger simulation. Part of the estimation for the time needed to follow particles depends on the total number emitted, how many are needed to simulate the dynamics of spacecharge limiting, and how many will have a long lifetime in the simulation. [Ultimately, the rules of thumb for selecting particle controls can be automated as well].

For the test computer, a 400 Hz Pentium II running nights and weekends, the target was less than a million for the average number of particles in space. Two simulations were run, using the same input except for increasing the particle emission by a factor of 3 for the second run. Typical results are compared in Figures 11 through 14.

Figure 11 shows the evolution of the number of particles in space. One expects the best simulation from starsat 3, which has up to 900k particles in space. As Figure 12 illustrates, both simulations successfully compute the electric field in the emission region on top of the satellite. However, the poorer particle statistics mar the prediction for the magnetic

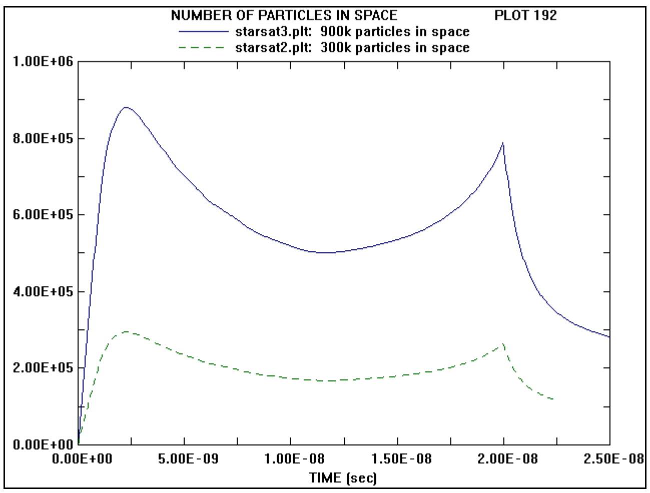

Figure 11. MEEC diagnostic output of the number of particles in space (peaks at time to spacecharge limit)

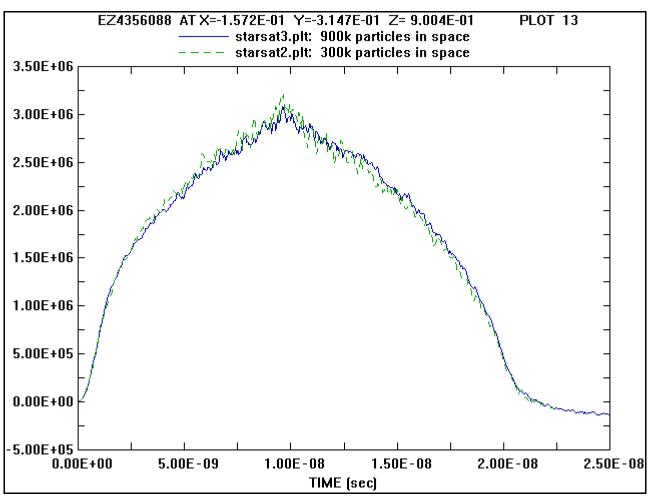

Figure 12. SGEMP Electric field on top of the center body computed by the test simulations.

field at the edge of the emission region, as shown in Figure 13. The dashed lines corresponding to few particles in the simulation show a much "noisier" field. Another SGEMP output response of interest, the current driven on the solar panel boom (Figure 14), appeared to be adequately simulated adequately in both runs.

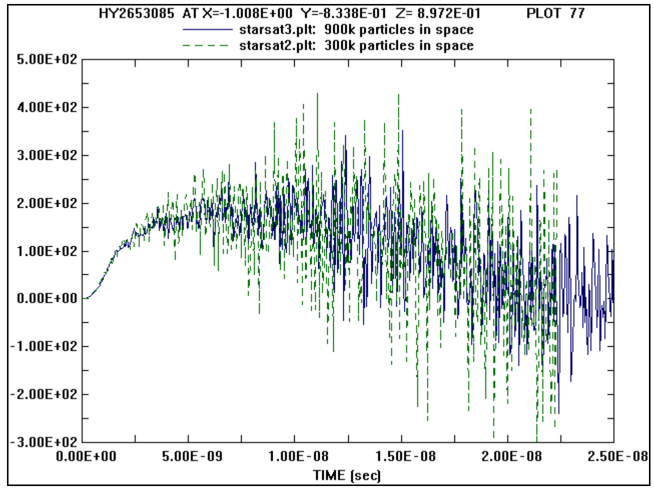

Figure 13. Surface magnetic field, indicating a better simulation (fewer high frequency spikes) with more particles.

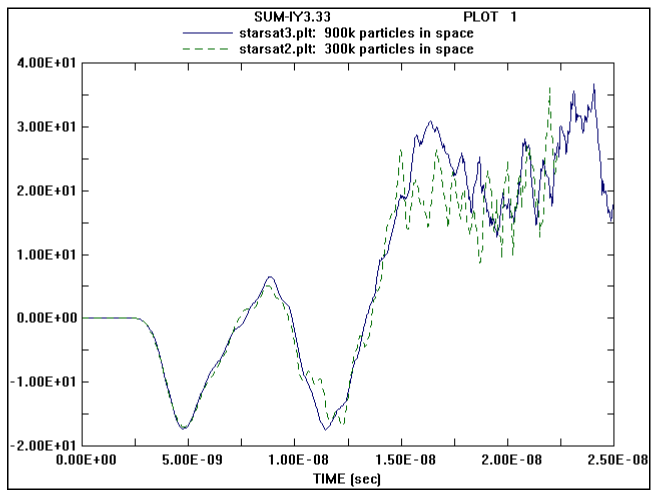

Figure 14. Boom current near the center body was reasonably simulated in both runs.

An approximation used in MEEC in the update of the fields based on particle currents works well when there are many particles per cell in the source region, but gets quite poor when too few particles are used. Therefore, simulation outputs in the SGEMP source region still need to be closely monitored to ensure a good simulation.

The results of this automated SGEMP simulation indicate success at basic geometry definition, if not at present all of the input.

SUMMARY AND CONCLUSIONS

This paper has described the development of a preliminary GUI and grid generator to produce the critical input for the MEEC SGEMP and SREMP codes. The intent has been to speed the modeling process by providing basic visualization tools and to prevent errors by automating what had been a tedious manual generation of objects and mesh. Also, some SGEMP analyst experience has been included in the choices and criteria used to cast objects onto a mesh and to choose the mesh size based on the SGEMP physics that needs to be accurately resolved. This "automation" of SGEMP simulation does not take the place of analyst insight into model inputs and interpretation of the results. It should, however, increase the reliability of basic input construction and provide simple error checks for complex simulation geometries.

REFERENCES

1. T. Tumolillo, “PRES-3D: A Computer Code for the Self-consistent Solution of the Maxwell-Lorentz Three-species Air-chemistry Equations in Three-dimensional Cartesian Coordinates”, December 1977.
2. T. Tumolillo, and J. Wondra, "MEEC-3D: A Computer Code for the Self-Consistent Solution of the Maxwell-Lorentz Equations in Three Dimensions," IEEE Trans. Nuc. Sci., NS-24 December 1977.
3. Rod Stephens, Visual Basic Graphics Programming, John Wiley & Sons, Inc. 1997.
4. CEPXS/ONEBFP is a code module contained within BOXIEMP II [Walters, J. Wondra, W. Seidler, L.J. Lorence, J.E. Morel, W. Walters, F. Brinkley, "Users' Handbook for BOXIEMP II - A Gamma Ray Transport, Photocompton Emission and IEMP Coupling Code", Release 1.2, JAYCOR Report J205-91-0195/2703, July 1992].
5. Carron, N. J. and C. L. Longmire, "Scaling Behavior of the Time-Dependent SGEMP Boundary Layer," IEEE Trans. Nuc. Sci., Vol. NS25, No. 6, December 1978